A High-accuracy Limited-range Equation of State for Liquid Sodium

Eric Chisolm, T-1

A major focus of the equation of state (EOS) program in the past has been the production of EOS that cover very wide spans of compression and temperature and that have physically sensible behavior over the entire range, particularly the limits of extreme conditions. The SESAME library, maintained at LANL for many decades, epitomizes this approach. However, more modern applications such as the simulation of nuclear reactors require a different emphasis: the EOS need cover only a few thousand kelvin and a few atmospheres of pressure, but its predictions of thermodynamic properties must be exceedingly accurate in that range. We have made recent advances in the production of EOS to meet these needs, as illustrated by a new liquid sodium EOS that is valid up to roughly 1100 K and ten atmospheres and reproduces experimental data to a few percent. Such an EOS is required for the study of proposed reactors that use sodium as a coolant.

The goal was to find relations for energy E and pressure P as functions of density ρ and temperature T in the required regions. The available data consisted of the density ρ, constant-pressure specific heat C_P, thermal expansion coefficient β, and isothermal bulk modulus B_T, all as functions of temperature at a fixed pressure of one atmosphere. The EOS was constructed in two stages. First the energy at a pressure of one atmosphere was constructed by integrating the thermodynamic identity:

$$\left(\frac{\partial E}{\partial T}\right)_P = C_P - \frac{\beta P}{\rho}$$

which required all of the experimental data except for the bulk modulus. This determined the entire EOS at one atmosphere. To calculate the EOS off the isobar, we started with the expression:

$$P(\rho,T) = P^{iso}(T) + \frac{B_T^{iso}(T)}{\rho^{iso}(T)}\left(\rho - \rho^{iso}(T)\right)$$

where the quantities with the superscript “iso” are given by the experimental data along the one atmosphere isobar. It is at this point that the isothermal bulk modulus is needed. This equation is not exact, but only an approximation valid at densities close to the isobar; it is here that we take advantage of the fact that the EOS is to be used only at low pressures. We integrated this expression to find the Helmholtz free energy F, and from there we calculated the energy E. The final expressions are complicated and may be found, with further supporting details, in [1]. Since we used an approximation for pressure, we needed to estimate its accuracy, concluding that the EOS is accurate to better than 5% in its least accurate form (and 0.5% in its most accurate form; see [1]) to pressures of 10 atmospheres.

We anticipate a greater demand for EOS of this type as more accurate simulations over smaller ranges of conditions become more important in nuclear energy and other applications.

For further information contact Eric Chisolm at echisolm@lanl.gov.

[1] Eric Chisolm, “A high-accuracy limited-range equation of state for liquid sodium,” Los Alamos National Laboratory report LA-UR-06-6668.

Funding Acknowledgments
- Department of Energy, Global Nuclear Energy Partnership